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Journal of Computational and Applied Mathematics 169 (2004) 247–254
JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS
www.elsevier.com/locate/cam

On the number of nodes in n-dimensional cubature formulae of degree 5 for integrals over the ball

M.V. Noskov[a,1], H.J. Schmid[b,*]

[a] *Department of Applied Mathematics, Krasnoyarsk State Technical University, Kirenskogo 26, Krasnoyarsk 660074, Russia*

[b] *Mathematisches Institut, Universität Erlangen-Nürnberg, Bismarckstrasse 1 1/2, Erlangen D-91054, Germany*

Received 21 July 2003; received in revised form 2 December 2003

Abstract

In this note cubature formulae of degree 5 are studied for n-dimensional integrals over the ball with constant weight function. We apply the method of reproducing kernel to show that the existence of such formulae attaining the best known lower bound is equivalent to the existence of tight spherical 5-designs. The known results concerning spherical 5-designs show that the lower bound for the integral under consideration will not be attained in general. The bound will be attained for $n=2,3,7,23$ and possibly for $n=(2\rho+1)^2-2$, $\rho \geqslant 5$. In all other cases the bound must be increased at least by 1, in particular, Stroud's formulae for $n=4,5,6,7$ are minimal.

Keywords: Cubature; Multivariate integrals; Spherical designs

1. Introduction

We denote the n-dimensional ball and sphere by

$$\mathscr{B}_n = \{X \in \mathbb{R}^n : \|X\|_2^2 \leqslant 1\}, \qquad \mathscr{S}_{n-1} = \{X \in \mathbb{R}^n : \|X\|_2^2 = 1\}$$

and consider the centrally symmetric integral

$$I_{\mathscr{B}}[f] = \frac{1}{V}\int_{\mathscr{B}_n} f(x_1,x_2,\ldots,x_n)\,\mathrm{d}x_1\mathrm{d}x_2\cdots\mathrm{d}x_n = \frac{1}{V}\int_{\mathscr{B}_n} f(X)\,\mathrm{d}X, \qquad V = \int_{\mathscr{B}_n} 1\mathrm{d}X,$$

* Corresponding author. Fax: +49-9131-852-2684.
E-mail address: schmid@mi.uni-erlangen.de (H.J. Schmid).

[1] The author was supported by the DAAD for a research stay in Erlangen.

0377-0427/$ - see front matter
doi:10.1016/j.cam.2003.12.024

satisfying $I_{\mathscr{B}}[1] = 1$. Denoting by $\mathbb{P}_m^n$ the linear space of real polynomials in n variables of total degree $\leqslant m$ the algebraic cubature problem for $I_{\mathscr{B}}$ can be stated as follows: Find N nodes $Q_i = (q_{i,1}, q_{i,2}, \dots, q_{i,n}) \in \mathscr{B}_n$ and N coefficients $C_i > 0$ such that

$$I_{\mathscr{B}}[f] = \sum_{i=1}^{N} C_i f(Q_i) \quad \text{for all } f \in \mathbb{P}_m^n$$

and

$$I_{\mathscr{B}}[g] \neq \sum_{i=1}^{N} C_i g(Q_i) \quad \text{for at least one } g \in \mathbb{P}_{m+1}^n.$$

If for fixed m the number of nodes N is minimal, the obtained cubature formula is called minimal. The best known lower bound for the number of nodes for formulae of degree $m = 2k+1$ for the integral considered is given by

$$N \geqslant 2\dim \mathbb{L}_k - \begin{cases} 1 & \text{if } \mathbf{0} \text{ is a node and } k \text{ is even,} \\ 0 & \text{else,} \end{cases}$$

where $\mathbb{L}_k$ is the subspace of $\mathbb{P}_m^n$ consisting of all polynomials having the same parity as k. This bound is due to Möller [11] and Mysovskikh [12]. Möller proved in addition that formulae attaining the bound in the first case are centrally symmetric. In the following we will restrict ourselves to the bound:

$$N \geqslant 2\dim \mathbb{L}_k - 1, \quad \mathbf{0} \text{ is a node and } k \text{ is even.} \tag{1}$$

We study cubature formulae of degree $m = 5$ in n dimensions with $N = n^2 + n + 1$ nodes such that N attains the lower bound (1). By applying the method of reproducing kernel the non-zero nodes of such a formula—if it exists—are distributed on a sphere with radius $(n+2)/(n+4)$ and have the same coefficient. Furthermore the nodes on the sphere form a tight spherical 5-design if we blow up the sphere to radius 1. The results known for spherical 5-designs can be applied straightforward.

Integrals are known for which even the simplest lower bound, $N \geqslant \dim \mathbb{P}_{[m/2]}^n$,—known from Gaussian quadrature—will be attained in every dimension and for each degree of exactness m (see [4]). Nevertheless, it is the common feeling that all known lower bounds for the number of nodes in cubature formulae do not hold in general (in particular for integrals over classical regions). Furthermore, most of the results which improved lower bounds were obtained by showing that methods based on characterizing theorems fail, see e.g. [7,17]. Our result has the same disadvantage. In [21] it is shown that integrals over $\mathscr{B}_n$ do not attain the lower bound for an arbitrary, but high degree of exactness. In this note it will be shown that even for degree 5 the bound is depending on n in a strange form.

2. Reproducing kernels

We will use the method of reproducing kernel to construct formulae for $I_{\mathscr{B}}$ attaining the lower bound. For an overview of this and other construction methods, see [6,13].

Due to the central symmetry of $I_{\mathscr{B}}$ cubature of formulae of degree $m = 2k + 1$, k even, which attain the lower bound (1), can be rewritten as

$$I_{\mathscr{B}}[f] \approx 2C_0 f(Q_0) + \sum_{i=1}^{(N-1)/2} C_i[f(Q_i) + f(-Q_i)], \quad Q_0 = \mathbf{0}, \tag{2}$$

where $N = 2\dim \mathbb{L}_k - 1$.

The reproducing kernel for $\mathbb{L}_k$ is defined by the property

$$f(X) = \int_{\mathscr{B}_n} f(Y)K(X,Y)\,\mathrm{d}Y \quad \text{for all } f \in \mathbb{L}_k.$$

We make use of the following.

Theorem 1. *A cubature formula* (2) *for* $I_{\mathscr{B}}$ *of degree* $m = 2k + 1$, k *even, with* $N = 2\,dim\,\mathbb{L}_k - 1$ *exists, if and only if*

$$K(Q_i, Q_j) = 0 \quad \textit{for all } i, j = 0, 1, 2, \ldots, (N-1)/2, \ i \neq j.$$

Furthermore, if the formula exists, then

$$C_i = \tfrac{1}{2} K(Q_i, Q_i)^{-1}, \quad i = 0, 1, \ldots, (N-1)/2.$$

For a proof and further references see [13]. The reproducing kernel can be constructed as follows: If

$$\Phi(X) = (\varphi_1(X), \varphi_2(X), \ldots, \varphi_\rho(X))$$

is a basis of $\mathbb{L}_k$ and if the Gram matrix for $I_{\mathscr{B}}$ with respect to Φ will be denoted by G, then

$$K(X,Y) = \Phi(X)G^{-1}\Phi^t(Y).$$

3. The reproducing kernel for degree 5

We study cubature formulae of degree $m = 5$ in n dimensions with N nodes, attaining the lower bound $N = n^2 + n + 1$ by applying Theorem 1. For $n = 2$ such a formula of degree 5 with 7 nodes has been constructed by Radon [14]. The case $n = 3$ with 13 nodes is due to Stroud [19]. The reproducing kernel for formulae of degree 5 involves only even degree polynomials of degree $\leqslant 2$, hence $\dim \mathbb{L}_k = (n^2 + n + 2)/2$.

An elegant representation of this kernel is given in [20, p. 164] for integrals over $\mathscr{B}_n$ with classical weight functions. In the formula [has to be replaced by [(and 2(μ by (2μ. Setting $\mu = \frac{1}{2}$ and $d = n$ the kernel for our constant weight function reads as follows:

$$\begin{aligned} K(X,Y) = {} & 2\lambda(\lambda+1)(X^tY)^2 + \lambda(\lambda+1)\|X\|_2^2\|Y\|_2^2 \\ & - \lambda(\lambda+1)(\|X\|_2^2 + \|Y\|_2^2) + \lambda^2 \end{aligned}$$

with

$$\lambda = \frac{n+2}{2}.$$

From this we get

$$K(X,\mathbf{0}) = \lambda^2 - \lambda(\lambda+1)\|X\|_2^2 = \frac{(n+2)(n+4)}{4}\left(\frac{n+2}{n+4} - \sum_{i=1}^n x_i^2\right).$$

So, whenever $Q \neq \mathbf{0}$ is a node of (2), then $K(Q,\mathbf{0}) = 0$, i.e.

$$\sum_{i=1}^n q_i^2 = \frac{n+2}{n+4}.$$

Hence all nodes—except node $\mathbf{0}$—lie on the sphere

$$\mathscr{S}_{n-1}^{\star} = \left\{X \in \mathbb{R}^n : \|X\|_2^2 = \frac{n+2}{n+4}\right\}.$$

It will turn out that the following modified form of the kernel for all nodes on the sphere is useful:

$$K^{\star}(X,Y) = K(X,Y) - \frac{1}{\lambda+1}\left(\frac{1}{\lambda}K(X,\mathbf{0})K(\mathbf{0},Y) + (K(X,\mathbf{0}) + K(\mathbf{0},Y))\right).$$

If $Q,P \neq \mathbf{0}$ are distinct nodes then $K^{\star}(Q,P)$ vanishes, and $K^{\star}(Q,Q) = K(Q,Q)$.

Since

$$K(X,\mathbf{0})K(\mathbf{0},Y) = \lambda^4 - \lambda^3(\lambda+1)(\|X\|_2^2 + \|Y\|_2^2) + \lambda^2(\lambda+1)^2\|X\|_2^2\|Y\|_2^2$$

we obtain

$$K(X,Y) - \frac{1}{\lambda(\lambda+1)}K(X,\mathbf{0})K(\mathbf{0},Y)$$

$$= 2\lambda(\lambda+1)(X^tY)^2 - \lambda(\|X\|_2^2 + \|Y\|_2^2) + \frac{\lambda^2}{\lambda+1}.$$

From

$$\frac{1}{\lambda+1}[K(X,\mathbf{0}) + K(\mathbf{0},Y)] = \frac{2\lambda^2}{\lambda+1} - \lambda(\|X\|_2^2 + \|Y\|_2^2)$$

we finally get

$$\begin{aligned} K^{\star}(X,Y) &= K(X,Y) - \frac{1}{\lambda(\lambda+1)}K(X,\mathbf{0})K(\mathbf{0},Y) \\ &\quad - \frac{1}{\lambda+1}(K(X,\mathbf{0}) + K(\mathbf{0},Y)) \\ &= 2\lambda(\lambda+1)(X^tY)^2 - \frac{\lambda^2}{\lambda+1} \\ &= \frac{(n+2)(n+4)}{2}\left((X^tY)^2 - \frac{n+2}{(n+4)^2}\right). \end{aligned}$$

For all $Q \in \mathscr{S}_{n-1}^{\star}$

$$K^{\star}(Q,Q) = \frac{(n+2)(n+4)}{2}\left(\left(\frac{n+2}{n+4}\right)^2 - \frac{n+2}{(n+4)^2}\right) = \frac{(n+2)^2(n+1)}{2(n+4)}.$$

Since the coefficient for a node $Q \neq \mathbf{0}$ of the cubature formula is given by

$$C_Q = \tfrac{1}{2}(K(Q,Q))^{-1} = \tfrac{1}{2}(K^{\star}(Q,Q))^{-1},$$

all nodes $Q \neq \mathbf{0}$ have the same coefficient

$$C_Q = \frac{n+4}{(n+2)^2(n+1)}. \tag{3}$$

The coefficient for the zero-node is

$$2C_{\mathbf{0}} = \frac{4}{(n+2)^2}.$$

This proves the following.

Theorem 2. *A cubature formula of degree* 5 *for $I_{\mathscr{B}}$ with a number of nodes attaining the lower bound* (1)*—if it exists—is of the form*

$$\frac{4}{(n+2)^2} f(\mathbf{0}) + \frac{n+4}{(n+2)^2(n+1)} \sum_{i=1}^{n(n+1)/2} [f(Q_i) + f(-Q_i)], \quad Q_i \in \mathscr{S}^{\star}_{n-1}. \tag{4}$$

4. Connection to spherical 5-designs

A finite set $\{Q_i,\ i = 1,2,\dots,N\} \subset \mathscr{S}_{n-1}$ is called spherical t-design, if

$$\frac{1}{N}\sum_{i=1}^{N} f(Q_i) = I_{\mathscr{S}}[f] = \frac{1}{W}\int_{\mathscr{S}_{n-1}} f(X)\,\mathrm{d}X, \quad W = \int_{\mathscr{S}_{n-1}} 1\,\mathrm{d}X$$

for all polynomials $f \in \mathbb{P}^n_t$ (see [8]). Thus t-designs are the nodes of cubature formulae for $\mathscr{S}_{n-1}$ with equal coefficients.

For $t = 2s+1$ the following lower bound for the number of nodes in a spherical t-design is due to Delsarte et al. [8]

$$N \geqslant 2\binom{n+s-1}{n-1}.$$

A t-design is called tight, if this lower bound will be attained.

The nonvanishing moments for $I_{\mathscr{S}}$ and $I_{\mathscr{B}}$ are

$$I_{\mathscr{S}}[1] = 1, \quad I_{\mathscr{S}}[x_\nu^2] = \frac{1}{n}, \quad I_{\mathscr{S}}[x_\nu^4] = \frac{3}{n(n+2)}, \quad \nu = 1,2,\dots,n,$$

$$I_{\mathscr{S}}[x_\nu^2 x_\mu^2] = \frac{1}{n(n+2)}, \quad \nu,\mu = 1,2,\dots,n,\ \ \nu \neq \mu,$$

$$I_{\mathscr{B}}[1] = 1, \quad I_{\mathscr{B}}[x_\nu^2] = \frac{1}{n+2}, \quad I_{\mathscr{B}}[x_\nu^4] = \frac{3}{(n+2)(n+4)}, \quad \nu = 1,2,\dots,n,$$

$$I_{\mathscr{B}}[x_\nu^2 x_\mu^2] = \frac{1}{(n+2)(n+4)}, \quad \nu,\mu = 1,2,\dots,n,\ \ \nu \neq \mu.$$

Theorem 3. *Q_i, $i = 1,2,\ldots,n(n+1) \in \mathscr{S}^{\star}_{n-1}$ and $\mathbf{0}$ are the nodes of a minimal cubature formula (4) of degree 5 for $I_{\mathscr{B}}$ with a number of nodes attaining (1), if and only if*

$$\sqrt{\frac{n+4}{n+2}}Q_i, \quad i = 1,2,\ldots,n(n+1),$$

form a tight 5-design.

Proof. Let us denote by

$$Q_i = (q_{i,1}, q_{i,2}, \ldots, q_{i,n}), \quad i = 1,2,\ldots,N-1 = n(n+1),$$

the nodes on the sphere. The nonvanishing moments for $I_{\mathscr{B}}$ can be transformed as follows:

$$I_{\mathscr{B}}[1] = 1 = \frac{4}{(n+2)^2} + \frac{n+4}{(n+2)^2(n+1)}\sum_{i=1}^{N} 1 = \frac{1}{n(n+1)}\sum_{i=1}^{N} 1 = I_{\mathscr{S}}[1].$$

For $v = 1,2,\ldots,n$ we get

$$I_{\mathscr{B}}[x_v^2] = \frac{1}{n+2} = \frac{n+4}{(n+2)^2(n+1)}\sum_{i=1}^{N} q_{v,i}^2.$$

Multiplying this by $(n+2)/n$ we get

$$\frac{1}{n} = I_{\mathscr{S}}[x_v^2] = \frac{1}{n(n+1)}\sum_{i=1}^{N} \frac{n+4}{n+2} q_{v,i}^2.$$

Similarly, multiplying

$$I_{\mathscr{B}}[x_v^4] = \frac{3}{(n+2)(n+4)} = \frac{n+4}{(n+2)^2(n+1)}\sum_{i=1}^{N} q_{v,i}^4$$

by $(n+4)/n$ leads to

$$\frac{3}{n(n+2)} = I_{\mathscr{S}}[x_v^4] = \frac{1}{n(n+1)}\sum_{i=1}^{N} \left(\frac{n+4}{n+2}\right)^2 q_{v,i}^4.$$

Finally, for $v, \mu = 1,2,\ldots,n$, $v \neq \mu$,

$$\frac{1}{(n+2)(n+4)} = I_{\mathscr{B}}[x_v^2 x_\mu^2] = \frac{n+4}{(n+2)^2(n+1)}\sum_{i=1}^{N} q_{v,i}^2 q_{\mu,i}^2$$

can be written as

$$\frac{1}{n(n+2)} = I_{\mathscr{S}}[x_v^2 x_\mu^2] = \frac{1}{n(n+1)}\sum_{i=1}^{N} \left(\frac{n+4}{n+2}\right)^2 q_{v,i}^2 q_{\mu,i}^2.$$

Hence if Q_i, $i = 1,2,\ldots,N$ are the nodes of formulae of degree 5 for $I_{\mathscr{B}}$ then

$$\sqrt{\frac{n+4}{n+2}}Q_i$$

form a tight spherical 5-design and vice versa. □

For tight spherical t-designs, in particular 5-designs, we refer besides [8] to [1,2,15,16]. Important for this note is a result from [1] which goes back to a paper by Lemmens and Seidel [10]. Tight spherical 5-designs exist for $n = 2, 3, 7, 23$ and possibly for $n = (2\rho + 1)^2 - 2$, $\rho \geqslant 5$. The cases $\rho = 3, 4$ where excluded in [3]. In the appendix of that paper it is shown that an infinite number of further ρs can be excluded.

5. Minimal cubature formulae of degree 5 for $I_{\mathscr{B}}$

Using the results for spherical 5-designs we obtain the following lower bound for the number of nodes in a cubature formula of degree 5 for $I_{\mathscr{B}}$,

$$N \geqslant \begin{cases} n(n+1)+1 & \text{if } n = 1,2,3,\ n = (2\rho+1)^2 - 2,\ \rho \in \mathbb{N}, \\ n(n+1)+2 & \text{if } n = 4,5,6,\ 6 < n \neq (2\rho+1)^2 - 2. \end{cases}$$

This bound is sharp for $n = 1, 2, \ldots, 7$ and $n = 23$. We list one reference for each of the known minimal formulae (Table 1).

As a contribution to Cools' Encyclopedia of cubature formulae (see [5]), we remark that Stroud's formulae for $I_{\mathscr{B}}$ are minimal in the dimensions $n = 4, 5, 6, 7$, an elegant minimal formula for $n = 7$ can be derived from Reznick's tight 5-design [15] (Table 2).

Table 1

Minimal cubature of degree 5 for $I_{\mathscr{B}}$			Tight spherical 5-design	
Dimension	Nodes	See	Points	See
2	7	[14]	6	[8]
3	13	[19] S_3: 5-1	12	[8]
4	22	[19] S_4: 5-1	—	
5	32	[18]	—	
6	44	[18]	—	
7	57		56	[16]
23	553		552	[9,10]

Table 2

Minimal formula of degree 5 for $I_{\mathscr{B}}$, dimension 7

Weight	Nodes (57)								
A	(	0,	0,	0,	0,	0,	0,	0	)
B	(	$\pm a$,	$\pm a$,	0,	$\pm a$,	0,	0,	0	)
B	(	0,	$\pm a$,	$\pm a$,	0,	$\pm a$,	0,	0	)
B	(	0,	0,	$\pm a$,	$\pm a$,	0,	$\pm a$,	0	)
B	(	0,	0,	0,	$\pm a$,	$\pm a$,	0,	$\pm a$	)
B	(	$\pm a$,	0,	0,	0,	$\pm a$,	$\pm a$,	0	)
B	(	0,	$\pm a$,	0,	0,	0,	$\pm a$,	$\pm a$	)
B	(	$\pm a$,	0,	$\pm a$,	0,	0,	0,	$\pm a$	)

$A = 4/81$, $B = 11/648$, $a = \sqrt{3/11}$.

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